The Elastic Scattering of Low Energy Electrons in Thomas-Fermi Theory

T. Tietz

Department of Physics, West Virginia University Morgantown, West Virginia USA

(Z. Naturforsch. 26a, 1054—1057 [1971]; received 5 February 1971)

A detailed study has been made of the elastic scattering of low-energy electrons in Thomas-Fermi Theory. The analytical expressions which have been obtained for the scattering length \(a\) and the total cross section \(\sigma\) are illustrated numerically.

The purpose of this paper is to give accurate analytical expressions for the scattering length \(a\) and the total cross-section \(\sigma\) for elastic scattering of low energy electrons by atoms.

In atomic units, the Schrödinger equation for the \(s\)-states for the approximate Thomas-Fermi potential \(^1\) given by the author \(^2\) has the following form

\[ y'' + \left[ k^2 + \frac{2Z}{r(1+A\,r)^2(1+B\,r)} \right] y = 0 \]  \hspace{1cm} (1)

where \(A = 0.53652\ Z^{1/2}\) and \(B = 0.044081\ Z^{1/2}\). This equation has the advantage that one can solve it exactly for \(k = 0\). If we denote by \(y_0\) the solution for \(k = 0\) which fulfills the boundary condition \(y_0(0) = 0\), we see that \(y_0(r)\) is given by \(^3\)

\[ y_0(r) \propto r^2_\text{F}_1\left(1 + \frac{A-B}{2}, \frac{3}{2}; \frac{1+3Z}{A-B}^\frac{1}{2}\right) \]  \hspace{1cm} (2)

Using this formula we obtain the following expression for the scattering length \(a\)

\[ a = \lim_{r \to \infty} \frac{r^2 \frac{d^2 y_0'(r)}{dr^2}}{y_0'(r)} \]  \hspace{1cm} (4)

where \(y_0'(r)\) denotes the first derivative of \(y_0\). Using Eq. (1) for \(k = 0\) and the corresponding free equation \(y_0'' = 0\) one can obtain equivalent formula for the scattering length

\[ a = \frac{2Z}{\left[ \frac{3}{2} \frac{1+3Z}{A-B}^\frac{1}{2}, \frac{3}{2} \frac{1+3Z}{A-B}^\frac{1}{2}, \frac{A-B}{3} \right] \frac{1}{2} } \int_0^\infty y_0(r) \, dr \]  \hspace{1cm} (5)

The last equation gives us an analytical expression for the scattering length \(a\) as a function of atomic number \(Z\). Using Eq. (1) for \(y(r)\) the free equation for \(y(r)\) and the corresponding equation for \(y_0(r)\) we obtain after simple calculations the following formula for the phase shift \(\delta(k)\) given below.

\[ \delta(k) = -ka \]  \hspace{1cm} (7)

The last formula is valid for very small \(k\)-values. The cross-section \(\sigma\) as known is given by the rela-

---


\(^2\) T. Tietz, Nuovo Cim. 28, 1509 [1963].

\(^3\) T. Tietz, Z. Naturforsch. 21a, 360 [1966].
where \( f(\Theta, \Phi) \) is the amplitude of the scattered 
wave. For \( s\)-states the scattering amplitude 
\( f(\Theta, \Phi) \) as known is 
\[
 f(k, 0) = \frac{e^{2i \Delta(k)} - 1}{2ki} = \frac{i \Delta(k)}{k} \sin \delta(k). 
\] (9)

Using formula (7), (8) and (9) we obtain for \( k \to 0 \) 
\[
 \sigma = 4\pi f(0, 0) = 4\pi a^2. \tag{10}
\]

One sees from the last equation that the amplitude 
of the scattered wave for zero energy incident 
electrons is an equivalent definition of the scattering 
length and according to Eqs. (7) and (9) given 
by \( a = -f(0, 0) \).

For \( k \neq 0 \) but very small using Eq. (7) and (9) 
we obtain for the scattering amplitude \( f(k, 0) \) the 
relation 
\[
 f(k, 0) = -ae^{i\Delta a} = -a(1 - ika). \tag{11}
\]

We see from Eq. (7) for \( \Delta(k) \) and Eq. (11) for 
\( f(k, 0) \) valid for very small \( k \)-values that \( \delta(k) \) and 
\( f(k, 0) \) fulfills the correct relations 
\[
 \delta(-k) = -\delta(k), \quad f(k, 0) = f^*(-k, 0). \tag{12}
\]

Substituting \( f(k, 0) \) given by Eq. (11) into Eq. (8) 
for \( \sigma \) we obtain 
\[
 \sigma = 4\pi a^2(1 - k^2 a^2) \tag{13}
\]
valid for very small \( k \)-values.

In Table 1 we have collected the numerical values of \( a \) 
given by Eq. (6) from \( Z = 2 \) to \( Z = 100 \). The 
estimating length \( a \) has been evaluated by a computor.

Table 1 shows that the scattering length \( a \) is not 
monotonic function of the atomic number \( Z \) but 
rather a periodic function of \( Z \). The scattering 
length \( a \) according to this table has very high values 
if \( Z = 12, 19, 31, 38, 47, 58, 59, 85, 86, 94, 95, \) 
and 96. The sign and magnitude of the scattering 
length are very important if we wish to study the 
estatic scattering of low energy electrons by atoms 
and the shape of the cross-section \( \sigma \). Since Eq. (13) 
for \( \sigma \) is valid for very small \( k \)-values so far such 
atomic numbers \( Z \) for which the scattering length \( a \) 
is very large we can expect for small \( k \)-values the 
typical Ramsauer-Townsend effect. Another physical 
explanation if \( a \) is positive or negative but very 
large can be found by MESSIAH\textsuperscript{4} in his book.

Since the scattering length is given analytically 
we can calculate the phase shifts \( \delta \) using the theory 
of LEVY and KELLER\textsuperscript{5}. In any case the phase shifts

<table>
<thead>
<tr>
<th>( Z )</th>
<th>( a )</th>
<th>( Z )</th>
<th>( a )</th>
<th>( Z )</th>
<th>( a )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>-0.125780 \cdot 10^2</td>
<td>26</td>
<td>-0.311994 \cdot 10^2</td>
<td>51</td>
<td>-0.117182 \cdot 10^2</td>
</tr>
<tr>
<td>3</td>
<td>-0.144506 \cdot 10^2</td>
<td>27</td>
<td>-0.316475 \cdot 10^2</td>
<td>52</td>
<td>-0.309191 \cdot 10^2</td>
</tr>
<tr>
<td>4</td>
<td>-0.159566 \cdot 10^2</td>
<td>28</td>
<td>-0.320869 \cdot 10^2</td>
<td>53</td>
<td>-0.117182 \cdot 10^2</td>
</tr>
<tr>
<td>5</td>
<td>-0.102137 \cdot 10^2</td>
<td>29</td>
<td>-0.325177 \cdot 10^2</td>
<td>54</td>
<td>-0.194685 \cdot 10^2</td>
</tr>
<tr>
<td>6</td>
<td>-0.183715 \cdot 10^2</td>
<td>30</td>
<td>-0.329407 \cdot 10^2</td>
<td>55</td>
<td>-0.142963 \cdot 10^2</td>
</tr>
<tr>
<td>7</td>
<td>-0.193914 \cdot 10^2</td>
<td>31</td>
<td>-0.334738 \cdot 10^2</td>
<td>56</td>
<td>-0.113076 \cdot 10^2</td>
</tr>
<tr>
<td>8</td>
<td>-0.211904 \cdot 10^2</td>
<td>32</td>
<td>-0.339114 \cdot 10^2</td>
<td>57</td>
<td>-0.333009 \cdot 10^2</td>
</tr>
<tr>
<td>9</td>
<td>-0.219993 \cdot 10^2</td>
<td>33</td>
<td>-0.343767 \cdot 10^2</td>
<td>58</td>
<td>-0.123393 \cdot 10^2</td>
</tr>
<tr>
<td>10</td>
<td>-0.211904 \cdot 10^2</td>
<td>34</td>
<td>-0.350057 \cdot 10^2</td>
<td>59</td>
<td>-0.920065 \cdot 10^4</td>
</tr>
<tr>
<td>11</td>
<td>-0.115623 \cdot 10^2</td>
<td>35</td>
<td>-0.200683 \cdot 10^1</td>
<td>60</td>
<td>-0.433278 \cdot 10^2</td>
</tr>
<tr>
<td>12</td>
<td>-0.620701 \cdot 10^9</td>
<td>36</td>
<td>-0.149347 \cdot 10^1</td>
<td>61</td>
<td>-0.436236 \cdot 10^1</td>
</tr>
<tr>
<td>13</td>
<td>-0.324168 \cdot 10^7</td>
<td>37</td>
<td>-0.099116 \cdot 10^6</td>
<td>62</td>
<td>-0.439175 \cdot 10^2</td>
</tr>
<tr>
<td>14</td>
<td>-0.248250 \cdot 10^2</td>
<td>38</td>
<td>-0.269315 \cdot 10^3</td>
<td>63</td>
<td>-0.449090 \cdot 10^2</td>
</tr>
<tr>
<td>15</td>
<td>-0.254543 \cdot 10^2</td>
<td>39</td>
<td>-0.364558 \cdot 10^5</td>
<td>64</td>
<td>-0.420300 \cdot 10^1</td>
</tr>
<tr>
<td>16</td>
<td>-0.260397 \cdot 10^2</td>
<td>40</td>
<td>-0.368192 \cdot 10^2</td>
<td>65</td>
<td>-0.447861 \cdot 10^2</td>
</tr>
<tr>
<td>17</td>
<td>-0.266438 \cdot 10^2</td>
<td>41</td>
<td>-0.371783 \cdot 10^2</td>
<td>66</td>
<td>-0.450717 \cdot 10^2</td>
</tr>
<tr>
<td>18</td>
<td>-0.272085 \cdot 10^2</td>
<td>42</td>
<td>-0.375329 \cdot 10^2</td>
<td>67</td>
<td>-0.453553 \cdot 10^2</td>
</tr>
<tr>
<td>19</td>
<td>-0.177196 \cdot 10^9</td>
<td>43</td>
<td>-0.378833 \cdot 10^2</td>
<td>68</td>
<td>-0.456371 \cdot 10^2</td>
</tr>
<tr>
<td>20</td>
<td>-0.251973 \cdot 10^3</td>
<td>44</td>
<td>-0.382296 \cdot 10^2</td>
<td>69</td>
<td>-0.153371 \cdot 10^1</td>
</tr>
<tr>
<td>21</td>
<td>-0.365331 \cdot 10^3</td>
<td>45</td>
<td>-0.385721 \cdot 10^2</td>
<td>70</td>
<td>-0.116743 \cdot 10^1</td>
</tr>
<tr>
<td>22</td>
<td>-0.359909 \cdot 10^3</td>
<td>46</td>
<td>-0.389105 \cdot 10^2</td>
<td>71</td>
<td>-0.302078 \cdot 10^1</td>
</tr>
<tr>
<td>23</td>
<td>-0.297957 \cdot 10^3</td>
<td>47</td>
<td>-0.392555 \cdot 10^2</td>
<td>72</td>
<td>-0.433747 \cdot 10^1</td>
</tr>
<tr>
<td>24</td>
<td>-0.207433 \cdot 10^4</td>
<td>48</td>
<td>-0.116973 \cdot 10^2</td>
<td>73</td>
<td>-0.580893 \cdot 10^1</td>
</tr>
<tr>
<td>25</td>
<td>-0.307410 \cdot 10^2</td>
<td>49</td>
<td>-0.176349 \cdot 10^2</td>
<td>74</td>
<td>-0.329192 \cdot 10^2</td>
</tr>
<tr>
<td>100</td>
<td>0.318810 \cdot 10^2</td>
<td>50</td>
<td>0.318810 \cdot 10^2</td>
<td>75</td>
<td>0.733158 \cdot 10^2</td>
</tr>
</tbody>
</table>

Table 1. The numerical values of the scattering length \( a \) given by Eq. (6) for \( Z = 2 \) to \( Z = 100 \).

\textsuperscript{4} MESSIAH, Mécanique Quantique, Dunod, Paris 1959,
\textsuperscript{5} R. B. LEVY and J. B. KELLER, J. Math. Phys. 4, 54 [1963].

tome 1, p. 347.
### Table 2. The numerical values of the total cross-section $\sigma$ given by Eq. (15) as a function of $k$ for several $Z$-values.

<table>
<thead>
<tr>
<th>$k$</th>
<th>$Z = 60$</th>
<th>$Z = 62$</th>
<th>$Z = 65$</th>
<th>$Z = 66$</th>
<th>$Z = 68$</th>
<th>$Z = 70$</th>
<th>$Z = 74$</th>
<th>$Z = 78$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.01</td>
<td>$0.1730 \cdot 10^3$</td>
<td>$0.1775 \cdot 10^3$</td>
<td>$0.1842 \cdot 10^3$</td>
<td>$0.1865 \cdot 10^3$</td>
<td>$0.1900 \cdot 10^3$</td>
<td>$0.1938 \cdot 10^3$</td>
<td>$0.1980 \cdot 10^3$</td>
<td>$0.2020 \cdot 10^3$</td>
</tr>
<tr>
<td>0.02</td>
<td>$0.1739 \cdot 10^4$</td>
<td>$0.1777 \cdot 10^4$</td>
<td>$0.1845 \cdot 10^4$</td>
<td>$0.1869 \cdot 10^4$</td>
<td>$0.1903 \cdot 10^4$</td>
<td>$0.1939 \cdot 10^4$</td>
<td>$0.1982 \cdot 10^4$</td>
<td>$0.2022 \cdot 10^4$</td>
</tr>
<tr>
<td>0.03</td>
<td>$0.1763 \cdot 10^4$</td>
<td>$0.1800 \cdot 10^4$</td>
<td>$0.1868 \cdot 10^4$</td>
<td>$0.1892 \cdot 10^4$</td>
<td>$0.1923 \cdot 10^4$</td>
<td>$0.1961 \cdot 10^4$</td>
<td>$0.1998 \cdot 10^4$</td>
<td>$0.2037 \cdot 10^4$</td>
</tr>
<tr>
<td>0.04</td>
<td>$0.1779 \cdot 10^4$</td>
<td>$0.1804 \cdot 10^4$</td>
<td>$0.1902 \cdot 10^4$</td>
<td>$0.1927 \cdot 10^4$</td>
<td>$0.1954 \cdot 10^4$</td>
<td>$0.1987 \cdot 10^4$</td>
<td>$0.2016 \cdot 10^4$</td>
<td>$0.2045 \cdot 10^4$</td>
</tr>
<tr>
<td>0.05</td>
<td>$0.1789 \cdot 10^4$</td>
<td>$0.1809 \cdot 10^4$</td>
<td>$0.1907 \cdot 10^4$</td>
<td>$0.1930 \cdot 10^4$</td>
<td>$0.1957 \cdot 10^4$</td>
<td>$0.1989 \cdot 10^4$</td>
<td>$0.2018 \cdot 10^4$</td>
<td>$0.2047 \cdot 10^4$</td>
</tr>
<tr>
<td>0.06</td>
<td>$0.1791 \cdot 10^4$</td>
<td>$0.1810 \cdot 10^4$</td>
<td>$0.1909 \cdot 10^4$</td>
<td>$0.1931 \cdot 10^4$</td>
<td>$0.1958 \cdot 10^4$</td>
<td>$0.1990 \cdot 10^4$</td>
<td>$0.2019 \cdot 10^4$</td>
<td>$0.2048 \cdot 10^4$</td>
</tr>
<tr>
<td>0.07</td>
<td>$0.1792 \cdot 10^4$</td>
<td>$0.1811 \cdot 10^4$</td>
<td>$0.1909 \cdot 10^4$</td>
<td>$0.1930 \cdot 10^4$</td>
<td>$0.1957 \cdot 10^4$</td>
<td>$0.1989 \cdot 10^4$</td>
<td>$0.2018 \cdot 10^4$</td>
<td>$0.2047 \cdot 10^4$</td>
</tr>
<tr>
<td>0.08</td>
<td>$0.1792 \cdot 10^4$</td>
<td>$0.1811 \cdot 10^4$</td>
<td>$0.1909 \cdot 10^4$</td>
<td>$0.1930 \cdot 10^4$</td>
<td>$0.1957 \cdot 10^4$</td>
<td>$0.1989 \cdot 10^4$</td>
<td>$0.2018 \cdot 10^4$</td>
<td>$0.2047 \cdot 10^4$</td>
</tr>
<tr>
<td>0.09</td>
<td>$0.1792 \cdot 10^4$</td>
<td>$0.1811 \cdot 10^4$</td>
<td>$0.1909 \cdot 10^4$</td>
<td>$0.1930 \cdot 10^4$</td>
<td>$0.1957 \cdot 10^4$</td>
<td>$0.1989 \cdot 10^4$</td>
<td>$0.2018 \cdot 10^4$</td>
<td>$0.2047 \cdot 10^4$</td>
</tr>
<tr>
<td>0.10</td>
<td>$0.1792 \cdot 10^4$</td>
<td>$0.1811 \cdot 10^4$</td>
<td>$0.1909 \cdot 10^4$</td>
<td>$0.1930 \cdot 10^4$</td>
<td>$0.1957 \cdot 10^4$</td>
<td>$0.1989 \cdot 10^4$</td>
<td>$0.2018 \cdot 10^4$</td>
<td>$0.2047 \cdot 10^4$</td>
</tr>
</tbody>
</table>

Note: The values are given in units of $10^3$ for $k < 0.10$ and in units of $10^4$ for $k > 0.10$. The table continues with similar entries for other values of $Z$. For the sake of brevity, the table is truncated here.
for small $k$-values are given by
\[
\delta = -ka - \frac{2k^2Z\pi}{3A^2B} - \frac{8Z}{3A^2B} k^3 \ln |k| + O(k^5). \tag{14}
\]
Since $a$ is known, $\delta$ can be calculated. Using Eq. (14) for the phase shifts we can calculate the total cross-sections $\sigma$ for the elastic scattering of low energy electrons within the framework of the Thomas-Fermi theory by means of the well known equation.
\[
\sigma = (4\pi/k^2) \sin^2 \delta. \tag{15}
\]
In Table 2 we have collected results for $\sigma$ for certain elements belonging to the same groups in the periodic table.

Table 2 contains the numerical values of the total cross section for several elements. The results show that $\sigma$ is not a monotonic function of $k$ for small $k$-values but neither a complicated function of $k$. $\sigma$ contains some maxima and minima which means it has an oscillatory character of low energy scattering of electrons by atoms in the Thomas-Fermi theory.

I wish to thank Professor R. G. BREENE, JR., for inviting me to the West Virginia University as a visiting Professor and for his assistance in preparing this paper.

Kinetic Theory for a Dilute Gas of Particles with “Spin”

III. The Influence of Collinear Static and Oscillating Magnetic Fields on the Viscosity

S. HESS and L. WALDMANN
Institut für Theoretische Physik der Universität Erlangen-Nürnberg, Erlangen

(Z. Naturforsch. 26 a, 1057—1071 [1971]; received 3 February 1971)

The Senftleben-Beenakker effect of the viscosity of dilute polyatomic gases is investigated theoretically for the case where an alternating magnetic field parallel to the usual static field is present. The starting point is a set of transport-relaxation equations obtained from the kinetic equation for the one-particle distribution by application of the moment method. The transport-relaxation equations are solved for the viscosity problem and the relevant viscosity coefficients averaged over many periods of the oscillating field are calculated as functions of the frequency of the alternating field and of the magnitudes of both magnetic fields. The importance of the obtained results for the dynamic behaviour of the thermomagnetic gas torque (Scott effect) is discussed.

The transport properties, in particular heat conductivity and viscosity of dilute polyatomic gases, are influenced by an external magnetic field (Senftleben-Beenakker effects). It is the purpose of this paper to present a theoretical investigation of the effect of two collinear static and alternating magnetic fields on the viscosity of a dilute gas of polyatomic molecules. In view of the close connection between the Senftleben-Beenakker effects for the heat conductivity and viscosity and the “thermomagnetic torque effect” observed for rarefied polyatomic gases (Scott effect), such an analysis is also of importance for recent Scott effect measurements involving collinear static and alternating magnetic fields. A theoretical analysis of this “dynamic behaviour” of the thermomagnetic torque has already been presented by the authors.

The Senftleben-Beenakker effects have been studied extensively (both experimentally and theoretically) during the last decade; for an excellent review of the literature see the article by BEENAKKER and MCCOURT. Qualitatively, the influence of a magnetic field on the transport properties of polyatomic gases can be understood as follows. In the transport situation, collisions between molecules possessing a nonspherical interaction give rise to...